

Non-Markovian Fermionic Stochastic Schrödinger Equation for Open System Dynamics

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In this paper we present an exact Grassmann stochastic Schrödinger equation for the dynamics of an open fermionic quantum system coupled to a reservoir consisting of a finite or infinite number of fermions. We use this stochastic approach to derive the exact master equation for a fermionic system strongly coupled to electronic reservoirs. The generality and applicability of this Grassmann stochastic approach is justified and exemplified by several quantum open system problems concerning quantum decoherence and quantum transport for both vacuum and finite-temperature fermionic reservoirs. We show that the quantum coherence property of the quantum dot system can be profoundly modified by the environment memory.

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Introduction.— Quantum dynamics of electronic systems coupled to fermion (electrons) or boson (phonons) environments has recently attracted wide-spread interest in quantum transport, quantum computing, and nanoscience [1, 2]. For example, the size reduction of quantum devices in microelectronics requires controllable systems consisting of only a few electrons, where quantum coherence and quantum interference become dominant. In addition, quantum dots coupled to electrons of a metal is an interesting setup in quantum information processing where the quantum coherence of qubits is essential for many quantum algorithms to gain an exponential speed-up over their classical counterparts. In the case of quantum open systems immersed in a bosonic environment, a theoretical formalism for quantum open system dynamics was developed to provide a powerful tool in studying quantum systems in a non-Markovian regime [3–9]. This theory has extended the standard Markov quantum state diffusion [10] to the case involving strong system-environment interaction or structured environments. For a Markov fermionic environment, both the quantum state diffusion equation [10] and Lindblad master equations [11] can be used to describe quantum dynamics of the system of interest. However, for a generic non-Markovian fermionic environment, a stochastic theory analogous to the non-Markovian quantum state diffusion equation is still missing. The major theme of this Letter is to develop a non-Markovian stochastic theory of electronic systems coupled to a fermionic environment. As an illustration of the power of the stochastic approach developed here, we derive the exact master equations governing the reduced density operator of the electronic systems coupled to vacuum and finite-temperature reser-

voirs.

To begin, we consider a model involving an electronic system in contact with a single fermion reservoir, where the system anti-commute with the bath [12]. The generalization to two reservoirs (*e.g.*, source and drain) can be established in a similar way. With necessary modifications, the formalism is versatile enough to deal with stochastic gate potentials and nonlinear couplings. The total Hamiltonian for the system plus environment may be written as [1],

$$\hat{H}_{\text{tot}} = \hat{H}_S + \hat{H}_R + \hat{H}_I, \quad (1)$$

where \hat{H}_S is the Hamiltonian of the electronic system in the absence of the environment, H_R is the Hamiltonian for a fermionic reservoir; $\hat{H}_R = \sum_{\mathbf{k}\alpha} \hbar\omega_{\mathbf{k}} \hat{b}_{\mathbf{k}\alpha}^\dagger \hat{b}_{\mathbf{k}\alpha}$ where $\hat{b}_{\mathbf{k}\alpha}^\dagger, \hat{b}_{\mathbf{k}\alpha}$ are the fermionic creation and annihilation operators $\{\hat{b}_{\mathbf{k}\alpha}, \hat{b}_{\mathbf{k}'\alpha'}^\dagger\} = \delta_{\mathbf{k}\alpha, \mathbf{k}'\alpha'}$, and the interaction Hamiltonian H_I is given by

$$\hat{H}_I = \hbar \sum (t_{\mathbf{k}\alpha} \hat{L} \hat{b}_{\mathbf{k}\alpha}^\dagger + t_{\mathbf{k}\alpha} \hat{b}_{\mathbf{k}\alpha} \hat{L}^\dagger), \quad (2)$$

where \hat{L} is the system coupling operator and $t_{\mathbf{k}\alpha}$ are the coupling constants. Note that \hat{H}_S is an arbitrary Hamiltonian operator that may contain interaction terms for the system particles (*e.g.*, Coulomb interactions between two electrons). The coupling operator \hat{L} may, in general, be represented by a set of fermionic operators which are coupled to all the participating external agents such as the source and drain reservoirs.

The primary purpose of the present paper is to develop a systematic theory for the models described by (1) and (2), that are relevant to non-equilibrium statistical mechanics, Path-integral theory and quantum devices based on quantum dots and mesoscopic electronics [13–19]. In the framework of the stochastic Schrödinger equation (SSE), the state of the open quantum system is described by a stochastic pure state, which is generated by

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a stochastic process. For the fermionic environment, similar to the fermionic path integral, the fermionic stochastic theory will involve a Grassmann stochastic process. We show that the reduced density matrix of the system of interest can be reconstructed from the pure states by taking the statistical mean over the Grassmann noise. As such, in principle, the exact master equation governing the reduced density operator can be recovered from the SSE, as illustrated by several physically interesting models below. Compared with the bosonic case, it is more complex to recover the density matrix from the corresponding SSE due to fermionic features of the system and bath [20, 21].

Non-commutative stochastic Schrödinger equation (SSE) and master equation. —Consider the model described by the total Hamiltonian Eq. (1), in the interaction picture with respect to the fermionic reservoir it becomes (setting $\hbar = 1$), $\hat{H}_{\text{tot}}^I(t) = \hat{H}_S + (\sum_j t_j \hat{L}^\dagger \hat{b}_j e^{-i\omega_j t} + \text{h.c.})$, here the subscript $\mathbf{k}\alpha$ is suppressed as j . In order to trace out the environmental variables, we introduce the fermionic coherent states $|\xi_j\rangle$ which is defined as $\hat{b}_j|\xi_j\rangle = \xi_j|\xi_j\rangle$. Here, ξ_j is a Grassmann variable, satisfying $\{\xi_i, \xi_j\} = 0$, and $\{\xi_j, \hat{b}_j\} = \{\xi_j, \hat{b}_j^\dagger\} = 0$ [22]. As shown below, the derivations and results for fermionic SSE are more complex than the bosonic case. Using the fermionic coherent state, we define $|\psi_t(\xi^*)\rangle = \langle \xi | e^{i\hat{H}_R t} e^{-i\hat{H}_{\text{tot}} t} | \psi_{\text{tot}}(0) \rangle$ where $|\xi\rangle = |\xi_1\rangle \otimes |\xi_2\rangle \otimes \dots$ is a collective notation for the coherent state of the fermionic bath. Then, the non-commutative stochastic Schrödinger equation for the system of interest can be written as [21]

$$\partial_t |\psi_t(\xi^*)\rangle = -i\hat{H}_{\text{eff}} |\psi_t(\xi^*)\rangle, \quad (3)$$

where the effective Hamiltonian is

$$\hat{H}_{\text{eff}} = \hat{H}_S - i\hat{L}\xi_{b,t}^* - i\hat{L}^\dagger \int_0^t ds K(t, s) \overrightarrow{\delta}_{\xi_{b,s}^*} \quad (4)$$

where $\xi_{b,t}^* = -i\sum_k t_k e^{i\omega_k t} \xi_{b,k}^*$ is the Grassmann noise and the correlation function is $K(t, s) = \sum_k \frac{\partial \xi_{b,t}}{\partial \xi_{b,k}} \frac{\partial \xi_{b,s}^*}{\partial \xi_{b,k}^*} = \sum_k |t_k|^2 e^{-i\omega_k(t-s)}$. Note that our approach is applicable to arbitrary correlation functions for both Markov and non-Markovian cases.

Eq. (3) may serve as a fundamental equation for open electronic systems coupled to a fermionic environment. Crucial to the practical applications of Eq. (3) is to express the Grassmann functional derivative under the memory integral in (4) in terms of system operators [4–9]. In order to calculate the functional derivative in the stochastic Schrödinger equation, we introduce an operator called the fermionic \hat{Q} operator (similar to the \hat{O} operator in bosonic case) as,

$$\hat{Q}(t, s, \xi^*) |\psi_t(\xi^*)\rangle = \overrightarrow{\delta}_{\xi_s^*} |\psi_t(\xi^*)\rangle, \quad (5)$$

where the functional derivative is always assumed as left functional derivative throughout this paper. With this

definition, the effective Hamiltonian in Eq. (4) can be written as,

$$\hat{H}_{\text{eff}} = \hat{H}_S - i\hat{L}\xi_{b,t}^* - i\hat{L}^\dagger \hat{Q}, \quad (6)$$

where $\bar{Q}(t, \xi^*) = \int_0^t ds K(t, s) \hat{Q}(t, s, \xi^*)$. The stochastic equation is derived directly from the microscopic Hamiltonian without any approximation. It should be emphasized that the system Hamiltonian H_S and the coupling operator \hat{L} are entirely general. The evolution of the electronic system is governed by this non-commutative stochastic equation. Although the mathematical form of the equation is similar to the bosonic case, the behavior of the system can be different due to fermionic features of the environment [12].

From the consistency condition for the fermionic SSE $\overrightarrow{\delta}_{\xi_s^*} \partial_t |\psi_t(\xi^*)\rangle = \partial_t \overrightarrow{\delta}_{\xi_s^*} |\psi_t(\xi^*)\rangle$, the fermionic \hat{Q} operator satisfies the following equation,

$$\partial_t \hat{Q} = -i[\hat{H}_{\text{eff}}, \hat{Q}] - i\overrightarrow{\delta}_{\xi_s^*} (\hat{H}_{\text{eff}} - \hat{H}_S). \quad (7)$$

Once the fermionic \hat{Q} operator is determined, the SSE can be cast into a time-local stochastic equation with the Grassmann type noise. Note that the reduced density operator for the open fermionic system can be obtained by taking the statistical average over all the Grassmann trajectories,

$$\hat{\rho}_r = \int \mathcal{D}_g[\xi] \hat{P} \quad (8)$$

$$\hat{P} = \frac{1}{2} (|\psi_t(\xi^*)\rangle \langle \psi_t(-\xi)| + |\psi_t(\xi^*)\rangle \langle \psi_t(\xi)| + |\psi_t(\xi^*)\rangle^s \langle \psi_t(-\xi)|^s + |\psi_t(\xi^*)\rangle^s \langle \psi_t(\xi)|^s) \quad (9)$$

where $\mathcal{D}_g[\xi] = \prod_k d\xi_k^* \cdot d\xi_k e^{-\xi_k^* \cdot \xi_k}$ is the Grassmann Gaussian measure. The notation “ \sim ” stands for the transformation that change all the creation and annihilation operators to their additive inverse, and “ \sim^s ” means the transformation “ \sim ” is applied to the system of interest only. Note that the reconstruction of density operator in this sense is more complex than that in the case of bosonic bath [20]. Due to the anti-commutative features, the density matrix is composed of four different kinds of trajectories in Eq. (9). However, they can be generated by the same trajectory $|\psi_t(\xi^*)\rangle$ via transformations [21], so we will only consider $|\psi_t(\xi^*)\rangle$ in the following parts and use the shorthand notation $|\psi_t\rangle \equiv |\psi_t(\xi^*)\rangle$. Taking the time derivative and using the Novikov-type theorem for the Grassmann noise [21], we can derive the *formal* exact master equation as,

$$\partial_t \hat{\rho}_r = -i[H_S, \hat{\rho}_r] + \{ \int \mathcal{D}_g[\xi] [\bar{Q}\hat{P}, \hat{L}^\dagger] + \text{h.c.} \}, \quad (10)$$

The above derivation of SSE and master equation is only for the case of vacuum, in which we assume the system and environment are initially in the state $|\psi_{\text{tot}}(0)\rangle =$

$|\psi(0)\rangle_S \otimes |\text{vac}\rangle_R$. However, the finite temperature can be incorporated in our approach, as shown in the examples below [21].

In a special case wherein the fermionic \hat{Q} operator is independent of noise, the master equation Eq. (10) becomes a simpler form

$$\partial_t \hat{\rho}_r = -i[\hat{H}_S, \hat{\rho}_r] + [\bar{Q}\hat{\rho}, \hat{L}^\dagger] + \text{h.c.} \quad (11)$$

If we take the Markovian correlation function $K(t, s) = \Gamma\delta(t, s)$, the \bar{Q} operator reduces $\bar{Q} = \Gamma\hat{L}/2$, and the master equation will reduce to the standard Lindblad Markov master equation, $\partial_t \hat{\rho}_r = -i[\hat{H}_S, \hat{\rho}_r] + \Gamma/2[\hat{L}\hat{\rho}_r, \hat{L}^\dagger] + \text{h.c.}$

Many-fermion system coupled to a vacuum fermionic reservoir. — In the first example, we consider a many-fermion open system coupled to a fermionic bath initially in the vacuum state. The total Hamiltonian is $H_{\text{tot}} = \sum_{j=1}^N \Omega_j \hat{d}_j^\dagger \hat{d}_j + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_{j,k} t_{j,k} \hat{d}_j^\dagger \hat{b}_k + t_{j,k} \hat{b}_k^\dagger \hat{d}_j$, where \hat{d}_j and \hat{d}_j^\dagger ($j = 1$ to N) are the fermionic annihilation and creation operators for the fermions in the system, \hat{b}_k and \hat{b}_k^\dagger are the fermionic annihilation and creation operators for the bath. Here $\hat{H}_S = \sum_j \Omega_j \hat{d}_j^\dagger \hat{d}_j$, and the coupling operator is $\hat{L} = \sum_j \hat{d}_j$. Then, the fermionic SSE is given by

$$i\partial_t |\psi_t\rangle = \left(\sum_j \Omega_j \hat{d}_j^\dagger \hat{d}_j - i \sum_j \hat{d}_j \xi_{b,t}^* - i \sum_j \hat{d}_j^\dagger \bar{Q} \right) |\psi_t\rangle, \quad (12)$$

where the \hat{Q} operator is given by $\hat{Q} = \sum_i f_i(t, s) \hat{d}_i$. Substituting the \hat{Q} operator into the Eq. (7), we obtain the differential equation for the time-dependent coefficient $f_j(t, s)$ as $\frac{\partial}{\partial t} f_j(t, s) = i\Omega_j f_j(t, s) + \sum_{k=1}^N F_k(t) f_j(t, s)$ with the initial condition $f_j(t, s = t) = 1$. $F_j(t)$ is defined as $F_j(t) = \int_0^t K(t, s) f_j(t, s)$. Thus, the exact \hat{Q} operator is fully determined. Then one immediately obtains the exact master equation

$$\partial_t \hat{\rho}_r = -i[\hat{H}_S, \hat{\rho}_r] + \left\{ \left[\left(\sum_{j=1}^N F_j(t) \hat{d}_j \right) \hat{\rho}, \sum_{j=1}^N \hat{d}_j^\dagger \right] + \text{h.c.} \right\}. \quad (13)$$

We have shown that the SSE can be a power tool in deriving the exact master equation for an exactly solvable many-body system.

Single quantum dot (QD) coupled to a finite-temperature bath. — We consider a single QD interacting with a finite-temperature fermionic bath. In the standard Hamiltonian Eq. (1) and Eq. (2), $\hat{H}_S = \omega_0 \hat{d}^\dagger \hat{d}$ and $\hat{L} = \hat{d}$. It is known that the finite temperature model can be transformed into the vacuum case by introducing a fictitious bath “c” as [5, 9], $\hat{H}_C = -\sum_k \omega_k \hat{c}_k^\dagger \hat{c}_k$. By properly choosing the parameters of bath “c”, the combined bath “b+c” can be initially prepared in a pure state which can be transformed to vacuum, while the real bath “b” is prepared in the thermal state after tracing over the fictitious bath “c”, i.e., $\rho_b(0) = \text{Tr}_c[\hat{\rho}_{bc}(0)] = \exp[-\frac{\hat{H}_b - \mu \hat{N}}{k_B T}]/Z$

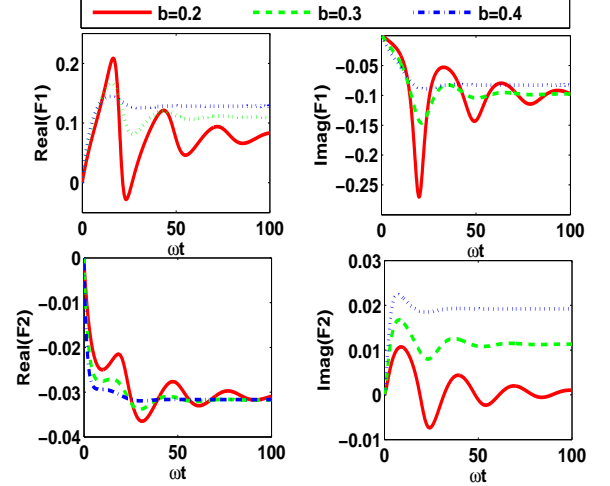


FIG. 1: Time evolution of the coefficients for single quantum dot in a finite temperature bath with different bandwidth. The real (imaginary) part of the coefficients F_1 (F_2) are plotted separately. The parameters are $T = 100mK$, $\mu = 2 \times 10^{-5}eV$, $\omega_0 = 3 \times 10^{-5}eV$.

where $Z = \text{Tr} \exp[-\frac{\hat{H}_b - \mu \hat{N}}{k_B T}]$ is the partition function. Therefore, the finite temperature model is transformed into an effective vacuum case with a fictitious bath [21]. Then, the exact SSE for the QD system is given by

$$i\partial_t |\psi_t\rangle = (\omega_0 \hat{d}^\dagger \hat{d} - i\hat{d}^\dagger \bar{Q}_{b'} - i\hat{d} \xi_{b',t}^* + i\hat{d}^\dagger \xi_{c',t}^* + i\hat{d} \bar{Q}_{c'}) |\psi_t\rangle \quad (14)$$

where the fermionic \hat{Q} operators are defined as $\bar{Q}_{b'} |\psi_t\rangle = \int_0^t ds K_{b'}(t, s) \vec{\delta}_{\xi_{b',s}^*} |\psi_t\rangle$, $\bar{Q}_{c'} |\psi_t\rangle = \int_0^t ds K_{c'}(t, s) \vec{\delta}_{\xi_{c',s}^*} |\psi_t\rangle$.

Following the scheme of deriving master equation from the general SSE, we obtain the exact master equation of this model,

$$\partial_t \hat{\rho}_r = -i[\hat{H}_S, \hat{\rho}_r] + \{F_1(t)[\hat{d}\hat{\rho}_r, \hat{d}^\dagger] + F_2(t)[\hat{\rho}_r \hat{d}, \hat{d}^\dagger] + \text{h.c.}\}, \quad (15)$$

The dynamic evolution is determined by the time-dependent coefficients. In the Markov limit, the coefficients are time-independent constants, however in the general non-Markovian case, the coefficients will be affected by the parameters of the environment. In Fig. 1, we plot the dynamic evolution of the coefficients $F_1(t)$ and $F_2(t)$. For simplicity, we choose noise-free \hat{Q} operator in our numerical simulations. The spectral density is chosen as the Lorentzian form $t_k^2(\omega_k) \Delta\omega = \frac{\Gamma b^2}{(1 - \frac{\omega_k}{\omega_0})^2 + b^2}$. When the bandwidth b is large, which corresponds to a white noise, then the coefficients converge to constants rapidly, approaching the Markov limit [18]. On the contrary, if the bandwidth b is narrow, the distribution of the spectral density represents a colored noise, then we

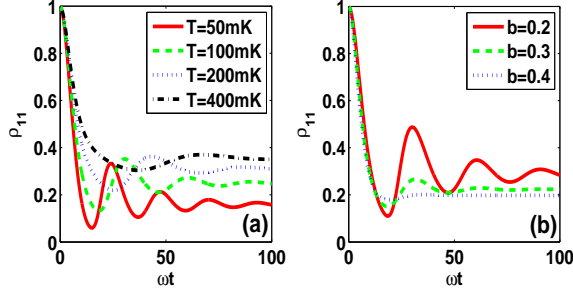


FIG. 2: Time evolution of ρ_{11} with different parameters of the bath. (a) is plotted with different temperature T , and (b) is plotted with different bandwidth of the spectral density. The other parameters are $\mu = 2 \times 10^{-5} \text{eV}$, $\omega_0 = 3 \times 10^{-5} \text{eV}$.

expect that the non-Markovian properties (e.g. time-dependent coefficients) will be observed. As a result, we see that in Fig. 2 (b), the density matrix element ρ_{11} converge to the steady state faster when the bandwidth b is larger, and it exhibits significant fluctuations when b is small.

Another parameter that will affect the non-Markovian properties is the temperature of the bath. As it is shown in Fig. 2 (a), the non-Markovian behaviors become apparent in the low temperature regimes and the Markov dynamics at high temperature.

Double QDs coupled to two finite-temperature fermionic baths – In the third example, we consider an electronic system coupled to two fermionic baths described by the following total Hamiltonian,

$$H_{\text{tot}} = \omega_1 \hat{d}_1^\dagger \hat{d}_1 + \omega_2 \hat{d}_2^\dagger \hat{d}_2 + g \hat{d}_1^\dagger \hat{d}_2 + g^* \hat{d}_2^\dagger \hat{d}_1 + \sum_k \omega_k (\hat{b}_{1,k}^\dagger \hat{b}_{1,k} + \hat{b}_{2,k}^\dagger \hat{b}_{2,k}) + \{ \sum_k t_{2,k} \hat{d}_2^\dagger \hat{b}_{2,k} + \sum_k t_{1,k} \hat{d}_1^\dagger \hat{b}_{1,k} + \text{h.c.} \}, \quad (16)$$

where \hat{d}_i and \hat{d}_i^\dagger ($i = 1, 2$) are the fermionic annihilation and creation operators for the two quantum dots in the system, and $\hat{b}_{i,k}$ and $\hat{b}_{i,k}^\dagger$ are the fermionic operators for the baths. This Hamiltonian describes a physical model that double quantum dots coupled to two fermionic baths, the “source” and the “drain”. This model is widely studied during the past few years with the input-output theory and fermionic path integral [19, 23].

In our SSE approach, following the similar procedure in example 2, the effective Hamiltonian of the model in the exact SSE can be established as

$$i\partial_t |\psi_t\rangle = (\hat{H}_S - i\hat{d}_1^\dagger \bar{Q}_{1,b'} - i\hat{d}_1^\dagger \xi_{1,b',t}^* + i\hat{d}_1^\dagger \xi_{1,c',t}^* + i\hat{d}_1 \bar{Q}_{1,c'} - i\hat{d}_2^\dagger \bar{Q}_{2,b'} - i\hat{d}_2^\dagger \xi_{2,b',t}^* + i\hat{d}_2^\dagger \xi_{2,c',t}^* + i\hat{d}_2 \bar{Q}_{2,c'}) |\psi_t\rangle \quad (17)$$

where $\bar{Q}_{\mu,\nu} |\psi_t\rangle = \int_0^t K_{\mu,\nu}(t,s) \overrightarrow{\delta}_{\xi_{\mu,\nu,s}^*} |\psi_t\rangle$ (the index $\mu =$

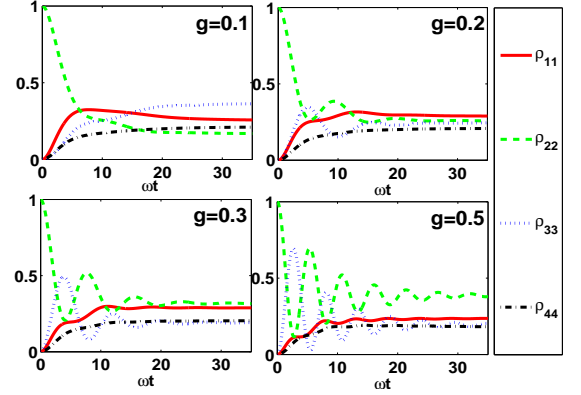


FIG. 3: Dynamic evolution for the initial state $d_1^\dagger |0\rangle$ with different coupling strength g . The other parameters are $T = 100 \text{mK}$, $\mu_1 = 2 \times 10^{-5} \text{eV}$, $\mu_2 = 4 \times 10^{-5} \text{eV}$, $\omega_1 = \omega = 2.5 \times 10^{-5} \text{eV}$, $\omega_2 = 3.5 \times 10^{-5} \text{eV}$.

1, 2 indicate the left and right baths, and $\nu = b', c'$ indicate the fictitious bath b' and c' in the finite temperature transformation). Therefore, the exact master equation for the double quantum dots system can be derived from the SSE,

$$\begin{aligned} \partial_t \hat{\rho}_r = & -i[\hat{H}_S, \hat{\rho}_r] + \{F_1(t)[\hat{d}_1 \hat{\rho}_r, \hat{d}_1^\dagger] + F_2(t)[\hat{\rho}_r \hat{d}_1, \hat{d}_1^\dagger] \\ & + F_3(t)[\hat{d}_2 \hat{\rho}_r, \hat{d}_1^\dagger] + F_4(t)[\hat{\rho}_r \hat{d}_2, \hat{d}_1^\dagger] \\ & + F_5(t)[\hat{d}_1 \hat{\rho}_r, \hat{d}_2^\dagger] + F_6(t)[\hat{\rho}_r \hat{d}_1, \hat{d}_2^\dagger] \\ & + F_7(t)[\hat{d}_2 \hat{\rho}_r, \hat{d}_2^\dagger] + F_8(t)[\hat{\rho}_r \hat{d}_2, \hat{d}_2^\dagger] + \text{h.c.}\}. \end{aligned} \quad (18)$$

The explicit expressions of the time dependent coefficients $F_i(t)$ ($i = 1$ to 8) can be found in [21]. Here, we show some simple properties of this model by plotting the time evolution of the population. The detailed study of this model will be discussed elsewhere [24]. In Fig. 3, we plot the dynamic evolution of the probabilities of all the states with different coupling strength between two dots. In a long-time limit, the system trends to converge to a steady state. When t is small, the electron tunneling from one dot to another can be significantly enhanced by the direct couplings between the two dots.

Conclusion.—In this letter, we develop the exact stochastic Schrödinger equation approach for solving the quantum open system coupled to a fermionic environment. The fundamental dynamic equation is derived directly from the microscopic quantum model without any approximations. By using the Grassmann noise, the stochastic Schrödinger equation approach is expanded from bosonic to fermionic environments. Three examples are presented to show the power of this approach. It is worth noting that the stochastic Schrödinger equation is versatile enough to deal with a generic fermionic

environment incorporating cases from a few fermions to an infinite number of fermions. The approach can be applied to more realistic systems when the approximation methods are used [24].

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